Dipropylamine 142-84-7 | DTXSID2025185

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Model	Data	

Weighted KNN model

5-fold CV (75	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.67

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 8.57e-01

Nearest Neighbors from the Training Set

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Dipropylamine Measured: 1.67 Predicted: 1.67

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1-Butanamine, N-propyl-

Measured: 2.12 Predicted: 2.12

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1-Butanamine, N-methyl-

Measured: 1.33 Predicted: 1.24

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2-Propanamine, N-ethyl-

Measured: 0.93 Predicted: 1.03